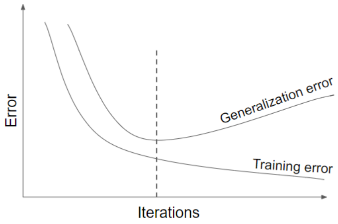
Introduction to Machine Learning

Regularization
Early Stopping



Learning goals

- Know how early stopping works
- Understand how early stopping acts as a regularizer
- Know early stopping imitates *L*2 regularization in some cases

EARLY STOPPING

- When training with an iterative optimizer such as SGD, it is commonly the case that, after a certain number of iterations, generalization error begins to increase even though training error continues to decrease.
- **Early stopping** refers to stopping the algorithm early before the generalization error increases.

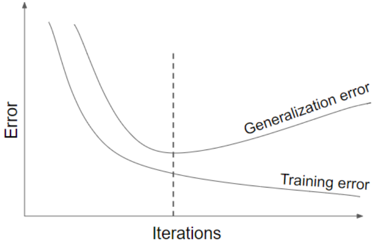
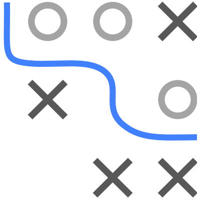


Figure: After a certain number of iterations, the algorithm begins to overfit.

EARLY STOPPING / 2



How early stopping works:

1. Split training data $\mathcal{D}_{\text{train}}$ into $\mathcal{D}_{\text{subtrain}}$ and $\mathcal{D}_{\text{val}}$ (e.g. with a ratio of 2:1).
2. Train on $\mathcal{D}_{\text{subtrain}}$ and evaluate model using the validation set $\mathcal{D}_{\text{val}}$.
3. Stop training when validation error stops decreasing (after a range of "patience" steps).
4. Use parameters of the previous step for the actual model.

More sophisticated forms also apply cross-validation.

EARLY STOPPING AND *L*2 ▸ Goodfellow, Bengio, and Courville 2016

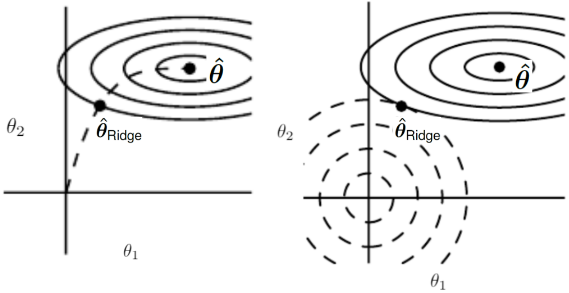
Strengths	Weaknesses
Effective and simple	Periodical evaluation of validation error
Applicable to almost any model without adjustment	Temporary copy of $\boldsymbol{\theta}$ (we have to save the whole model each time validation error improves)
Combinable with other regularization methods	Less data for training $\rightarrow$ include $\mathcal{D}_{\text{val}}$ afterwards

- For simple case of LM with squared loss and GD optim initialized at $\boldsymbol{\theta} = 0$: Early stopping has exact correspondence with *L*2 regularization/WD: optimal early-stopping iter T_{stop} inversely proportional to λ scaled by step-size α

$$T_{\text{stop}} \approx \frac{1}{\alpha\lambda} \Leftrightarrow \lambda \approx \frac{1}{T_{\text{stop}}\alpha}$$

- Small λ (regu. $\downarrow$) $\Rightarrow$ large T_{stop} (complexity $\uparrow$) and vice versa

EARLY STOPPING AND *L*2 ▸ Goodfellow, Bengio, and Courville 2016 / 2



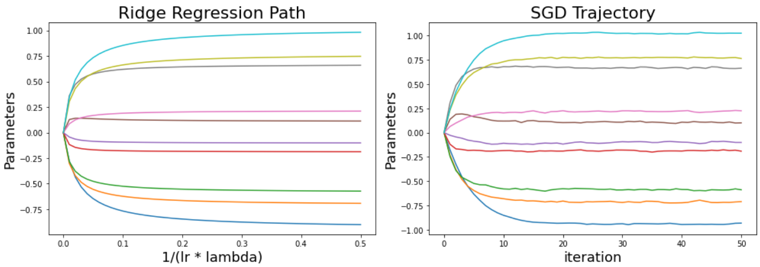
Goodfellow et al. (2016)

Figure: Effect of early stopping. *Left:* The solid lines indicate contours of the square loss objective. Dashed line indicates trajectory taken by GD initialized at origin. Instead of reaching minimizer $\hat{\theta}$, ES results in trajectory stopping earlier at $\hat{\boldsymbol{\theta}}_{\text{ridge}}$. *Right:* Effect of *L*2 regularization. Dashed circles indicate contours of *L*2 constraint which push minimizer of regularized cost closer to origin than minimizer of unregularized cost.

SGD TRAJECTORY AND *L2*

▸ Ali, Dobriban, and Tibshirani 2020

Solution paths for *L2* regularized linear model closely matches SGD trajectory of unregularized LM initialized at $\boldsymbol{\theta} = 0$



Caveat: Initialization at the origin is crucial for this equivalence to hold, which is almost never used in practice in ML/DL applications